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19. ABSTRACT (Continue on reverse if necessary and identify by block number) For the ultimate solution of the problem of "Chemisorption Under Stress" we have developed 1) a first principles theory for the calculation of the energy levels of solids as well as of aggregates of atoms that is analytically exact and computationally efficient giving the energy levels to unprecedented accuracy with a minimum of computational effort; 2) a first principles microscopic theory of Quantum Optics that gives the real time dynamical evolution of quantum states of individual atoms and shows how collective states develop; this theory not only reproduces the well known Quantum Optical phenomena for the first time in such detail and from one single theory but also predicts new bistable states that promise to be technologically very significant. We have also published in Statistical Mechanics that connect these findings to the topic of the grant. A list of publications is included.			
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of

Mikael Ciftan

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Abstract-Long Version

We have developed, under ARO support for which this FINAL REPORT is written, three major theories as necessary tools to attack the problem of "chemisorption of atoms and molecules onto stressed substrates" which in turn is responsible for a wide spectrum of phenomena such as the catastrophic failure of structures due to stress-corrosion cracking on one end of the spectrum and the control of crystalline imperfections during crystal growth in the opposite microscopic end of the spectrum. Our previous extensive work under ARO support had taught us that not only did we need a new and more precise method of calculating energy levels of solids and atoms but also to take care of the real time dynamics involved since chemisorption is a temperature dependent dynamical problem. Therefore we had to develop not only a new way of calculating energy levels (static, zero-temperature) but also develop a method that follows the real time evolution of states of the system immersed in a bath (finite temperature).

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Therefore under this ARO support we developed a fundamentally new first principles theory and computational method to calculate the energy levels of solids as well as of atoms or molecules; this new theory is free from the ad hoc assumptions of previous theories and is at the same time computationally much more efficient and more accurate than previous theories (giving all the energy levels at once and to extreme precision with a minimum of computation). We have published these results, both the theoretical framework and computational test cases that demonstrate the power of this new theory. The next steps in this development involve the introduction of a surface and thereafter the introduction of the adatom in order to calculate the static (zero-temperature) chemisorbed states.

In order to take account of the time evolution of the system we needed to develop a new fully rigorous first-principles quantum-mechanical microscopic theory, essentially solving the classic phase transition problem in real time and at the microscopic level but starting with a real Hamiltonian--surpassing the renormalization group and phenomenological methods. The best place to try this was in Quantum Optics not only because there was no such theory in Quantum Optics but also because in Quantum Optics we had a real and workable Hamiltonian that nobody could dispute. Using this as a testing ground we would then be able to attack the dynamics of chemisorption with chemisorption's own microscopic Hamiltonian. We therefore developed a new microscopic dynamical theory of Quantum Optics from first principles. It gives, for the first time, the atom-by-atom real-time dynamical evolution of quantum optical resonance phenomena. It allows one to correctly follow the time evolution of transient phenomena such as photon echoes and superradiance as well as steady state phenomena such as absorptive bistability within the same model by simply changing parameters. In addition to allowing one to probe the microscopic details of the first order phase transition exhibited by the latter system, it predicts the existence of new bistable states.

During the next two years of support under the new grant (Proposal No. 27424-PH) we shall fully investigate the prediction by this theory of these new bistable states. The initial investigations of this theory suggest that these new states may provide both the fastest optical switching mechanism possible and the highest spatial density of optical elements. If these hypotheses are confirmed, it would significantly impact emerging optical information processing technologies. We note that the theory we have developed also impacts theoretical physics itself by elucidating outstanding questions in quantum electrodynamics, the quantum theory of measurement, quantum statistical dynamics and especially the theory of critical phenomena.

We also give the rationale for our work in statistical physics that ties the above two endeavours to our initial problem of studying "chemisorption under stress." We give a historical account in the following section, "Introduction" and a thorough technical discussion after that. A complete list of papers published under recent ARO support is included at the end.

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I. Introduction

Under ARO support (Proposal no. _____ for which this FINAL REPORT is written) three major theories [6], [19], [18] were developed that have been well received internationally by the scientific community. We had developed these theories as precursors to our main problem of studying the dynamical phase transitions of chemisorbed atoms when the substrate is stressed. The first two of these theories (which constitute an exact generalized multiple scattering theory) we developed because it became clear to us that we needed a very accurate method of evaluating the self-consistent energy levels of the bulk (3-dimensional) crystalline solids, a solid with a surface to represent the substrate, the semi-infinite solid interacting with the adatoms, and finally the latter while stressing the substrate. We have tested the efficacy of our multiple scattering theory and have shown [13], [14] it to be highly accurate in test applications.

The third theory (our microscopic dynamical theory of quantum optics [18], [26]) appears at first sight to belong to a different branch of physics but in fact was developed to help us understand critical dynamics in an open system where the actual Hamiltonian was well-known. The chemisorption of adatoms onto a stressed substrate is a real-time, non-equilibrium dynamical process where "temperature" (insofar as it can be defined in an open, non-equilibrium system), local interactions, and non-Markovian effects all play an important role. Very little is known or understood about the best way to study systems of this sort in quantum statistical mechanics, where one usually *begins* to work by making the mean field, Markov, and zero-temperature approximations and, at best, attempts to restore corrections *a posteriori*.

The optical theory we developed in response to this difficulty is explicitly non-Markovian and allows the interactions to vary according to the location of an atom, its particular time-dependent state, and the time-dependent states of its neighboring atoms. Furthermore, it follows the microscopic optical trajectories of the constituent atoms through a representative of phase space *explicitly* and thus allows us to evaluate and observe the generalization of the notion of "temperature" for a non-equilibrium, open system. The spatial and temporal fluctuations of the system are directly calculable in "real-time" in this theory, as is their role in nucleating phase transitions. We directly calculate the actual time dependent state of a many atom system without recourse to statistical mechanics and its inevitable averages over significant information.

We now can calculate the zero-temperature energy level structure (band structure) of the substrate and the adatomic energy levels in the same (multiple scattering) theory and augment this zero temperature description by introducing non-Markovian local dynamics into the effective interaction Hamiltonian, using the general methodology developed in our theory of microscopic quantum optics.

We feel comfortable with the progress we have made in this second aspect of our problem. However, it turned out that there was a new richness in the microscopic solutions we obtained from our theory of optics that was not anticipated by any of the existing theories of optical resonance (which rely heavily on mean-field and Markov approximations). In particular, the application of our theory revealed new states not predicted by any other theory, as well as opening up previously hidden aspects of existing, supposedly well-understood phenomena. These new states and the new richness in the theory itself need investigation in their own right because of their implications to physics in general and to the technology of optical information processing in particular.

It is for this reason that we now want to further investigate the implications of our theory in quantum optics for the next two years, under the new staff research grant (Proposal No. 27424-PIT). Specifically we have shown that a new, and possibly the *fastest* and *smallest* optically bistable device may be developed based on our findings. We want the opportunity to explore in detail this new, and rather exciting, development.

II. History of Recent Research Under ARO Support

Let us briefly review our papers published under ARO support and the status of our research.

a. Multiple Scattering Theory

Our original paper on multiple-scattering band theory [6] was well received even by such luminaries as Prof. P. O. Löwdin (member of the Nobel Committee) and others at Sanibel [11]. This theory has been extensively studied in the literature by ourselves and others (see various references in the Bibliography) and is recognized and respected in the quantum chemistry community. We have given a number of invited papers on this subject, also listed in the Bibliography. Our research efforts on this subject have actively continued even while we were directing the bulk of our effort to the study of non-equilibrium dynamical optical systems. [19], [21], [22] have been published or in the last year in *Physical Review* and *Journal of Physics*, and an additional paper, [25], is under review.

This theory was derived by us because of our interest in developing a computationally accurate theory of chemisorption of atoms on surfaces. To improve on existing approaches it was clear to us that we needed to begin with a self-consistent description of the energy levels and wavefunctions in the bulk crystalline solid (of the substrate), add to this description a surface (modifying the bulk wavefunctions and creating surface states), evaluate the quantum chemical interaction of adsorbed species with this self-consistent substrate, and finally include the effects of dynamics, local symmetry

breaking and stress.

In our seminal paper on this subject we derived an *exact* solution to the first step in this problem, the computation of the energy levels and wavefunctions in the bulk solid. This solution generalized the "muffin-tin" approximated version of multiple scattering band theory (KKR band theory [28], [29]) to the case of arbitrary potentials. Among the advantages of this approach are that:

1. It does not require *ad hoc* assumptions concerning the potentials or relevant levels.
2. It yields the core levels intrinsically on the same footing as the valence bands.
3. It automatically accounts for any "hybridization" of the levels in complicated structures. The self-consistent wavefunctions it returns are automatically "mixed" by the non-spherically symmetric cell potentials.
4. It achieves highly accurate results (error < 0.01 eV) with very modest determinants.
5. It allows the quantum chemistry portion of the calculation to be performed *within the same formalism* (of multiple scattering theory, see below).

We have tested (and are still testing) this theory, both in a trial calculation of an actual metal and in the "empty lattice test". The results of our calculations to date, and other calculations that address our method, show that our theory is exact and extremely accurate (see Bibliography for numerous references).

The full chemisorption calculation also requires the evaluation of the chemical bonding between the adsorbed atom and the substrate. Multiple scattering theory has been used for many years (in a muffin-tin approximated form) to perform quantum chemistry calculations as the "scattered wave method" [31]. It became clear to us, during our studies of the generalized multiple scattering band theory, that a related generalization of multiple scattering theory existed that would *eliminate the muffin-tin approximation once and for all in both band theory and quantum chemistry*. We also realized that our original derivation could be simplified by rederiving the result from a much more fundamental starting point.

We therefore derived and published the equations for generalized multiple scattering theory [19], [23], [25] from a new point of view. These equations solve *exactly* the problem of finding the electronic states of atoms, molecules, or solids. In addition, they solve the general single and multiple scattering problem for non-electronic (e. g. - nuclear physics) problems. This new derivation is extremely straightforward and in fact

requires only two pieces of paper to fully describe. It proceeds from an easily proven identity and is *manifestly* exact. This theory will be a key ingredient in the final theory of chemisorption under stress.

At this point we had in our hands the basic elements of a static theory, and could have proceeded to do a static calculation. However, it was clear from both experimental and theoretical results that chemisorption under stress was a *dynamical* problem, and, furthermore, that defects played a critical role. We therefore turned our attention to non-equilibrium dynamics and critical phenomena to gain an understanding of how best to include these key ingredients. In our earlier studies of physisorption [1], [2], [3], [7] we used a known Hamiltonian and standard quantum statistical mechanics to evaluate the chemostress effect. This gave us a clear understanding of the essential ingredients of an exact theory, particularly for chemisorption (which involves quantum electronic interactions, bonding and many body effects). The latter paper [7] speculated about the non-linear effects of stress on external probes such as Raman scattering. This motivated a semi-phenomenological study of renormalization for systems with reduced dimensionality [16], [17].

From this work it became clear that traditional renormalization was incapable of resolving our difficulties because of the approximations inherent to the approach. Searching for alternatives, we decided to address the problem in the context of quantum optics, where the Hamiltonian of an open system was well known. Our initial research [8], [9] was somewhat disappointing because of the grave difficulties we encountered in our attempts to describe non-Markovian effects and local fluctuations in the traditional approaches. This motivated our fully microscopic investigation of this subject, which succeeded beyond our expectations and is the subject of work to be performed under the new staff research grant during the next two years. Our germinal work on optics has been presented and published [15], [20] and a full account of the theory has just appeared in *Physical Review A* 40, p. 3080 (Sept. 15, 1989) [26] and we are inundated with reprint requests.

We feel that in the next two years of support we will be able to demonstrate the theoretical feasibility of the new bistable states for optical devices. Concurrently we shall develop cooperative and collaborative efforts with experimentalists who can search for these effects in suitable materials.

b. Quantum Optics

Under the previous ARO contract (number DAAL03-87-0009) a microscopic theory of quantum optics was developed that can trace the evolution of the individual and collective atomic states in "real time". The equations we derive amount to a set of

“optical Bloch equations” for *each* independent atom in the system, coupled by the total reaction field (with the self-interaction term going into the spontaneous emission process as it should). Inhomogeneous dephasing processes are explicitly included in the equations of motion in a very general way. Homogeneous dephasing processes (like atom-atom elastic collisions) are also accounted for explicitly in a “unitarity preserving” way. Finally, spontaneous emission is accounted for, both at the level of the fundamental equations and in their c-number implementation, also in a unitarity preserving way.

These equations are implemented in a numerical computation according to an algorithm we have developed that allows us to study as many atoms as our computational resources allow — currently around $N = 600$. At this point most of the bulk phenomena are already well reproduced, and various schemes exist for extending our results to the large N limit. The equations we solve are of the Langevin type *for each atom* and explicitly account for field fluctuations and correlated fluctuations in the atomic states in a fully unitary manner. A single, particular solution of these stochastic differential equations is equivalent to a single trajectory through the phase space of possible trajectories for the many body system (and corresponds to a possible measurement of the actual system) or a single path in a Feynman path integral. It exhibits exactly the same fluctuations and stability that a particular experiment would, including all atom-field correlation functions through at least second order (indicating that it is a fully quantum mechanical result).

This theory correctly accounts for by now well established quantum optical phenomena such as photon echoes, self-initiating superradiance, free induction decay, and absorptive optical bistability from a *single* set of coupled equations derived rigorously from the quantum mechanical Hamiltonian for the atom-field interaction [18], [26]. We can study these different phenomena with a single set of equations by simply changing the dephasing rates and the spontaneous emission rate that describe the particular two-level atomic species, the “experimental situation” (such as the characteristics of an optical cavity and the spatial location of the atoms) and the applied “external field”, exactly as one would in an actual experiment. This alone sets the theory apart from existing models that obtain descriptions of at most one or two of these phenomena at the expense of completely neglecting or heavily approximating the effect of one or more of the dephasing mechanisms. Our model can be used to study systems with all the distinct kinds of dephasing occurring on arbitrary timescales.

In addition the solution to the model equations gives the details of the dynamics of the microscopic state of the atoms in the system that previous models cannot account for by their very nature. The existing model equations that are applied to resonance phenomena average over the behavior of the many atoms and obtain a *single* set of

equations for average quantities. The new theory yields instead *many* sets of coupled equations whose repeated solutions from a given set of initial conditions (with certain quantum stochastic elements) may be averaged if desired. Our major contribution to the theory of quantum optics is that we have deduced the correct way to incorporate the apparently non-unitary decay terms that appear in coupled many body equations into a fully unitary, microscopic dynamical description that preserves the essential quantum theory.

The present theory therefore reveals such sought for details as the true dynamical real-time evolution of an optical system as it undergoes a first order phase transition in absorptive bistability. "Critical slowing down", fluctuation-dissipation relationships, and the rates of transitions *away* from the critical points for finite systems are all directly observable in our solutions — all without resorting to extremally introduced schemes of renormalization. The dynamical equations themselves "decide" what their order parameters are and when and how to carry out the processes that are averaged over in renormalized non-linear dynamical theories. Especially useful is the ability to examine the stability of small N systems for which the theory of renormalization can intrinsically make no useful predictions. The critical role of non-Markovian processes (neglected in current treatments) in nucleating phase transitions is also clearly apparent in the dynamical solutions.

This theory also predicts the recently observed "photon locked" states that are the analogs of Redfield's spin locked states (where free induction decay is inhibited by the application of a detuned pulse and a strong resonant field [36], [37]). These states are ordinarily transient, with a lifetime determined by the homogeneous dephasing processes and spontaneous emission. By taking account of a local coupling between neighboring atoms in real space and real time (which is *possible* only in our model) and solving the dynamical equations to obtain a complete microscopic description we find that under certain circumstances *these states may become stable!* Switching between an opaque state or a transparent photon locked state or between the two photon locked states with opposite polarization is possible using nothing but appropriately detuned pulses.

This is a most significant result for the following reasons:

- In the case of absorptive bistability one must wait a certain amount of time, characteristically many times the dephasing lifetime, before the system becomes completely stable in its new state after driving it through a phase transition. This time is required for the system to "reorganize" its microscopic state into the new equilibrium configuration. This stabilization time fundamentally limits the minimum cycle time for such a switch and hence the rate at which an optical switch based processing unit could function. A photon locked switch does not require this

stabilization time because the initial and final states are homologous. Indeed, in the case of polarization switching they are symmetrical. A photon locked switch is limited in speed only by the spectral broadening of the short switching pulses, which is a fundamental limit in any optical resonance system of switches in any case. Even this limit is not absolute since frequency modulated switching may be possible at constant field amplitude.

- In the case of absorptive bistability one requires many atoms (and a high density of atoms) in a radiation trapping cavity to achieve the "cooperativity" required to stabilize the absorptive branch. Dispersive bistability has similar requirements, and the cavity in this case is essential to the bistability mechanism (cavity detuning) itself. A photon locked switch has similar requirements in order to be bistable in *transmittivity* but does *not* require a radiation trapping cavity to be bistable in *polarization*. Nor does a polarization switch require many atoms or a high density of atoms (although it *does* require a special *geometry* of atoms).

For these reasons, a phase locked polarization switch may be the fastest, smallest optical switch possible to construct out of "two-level" atoms. This clearly is of the greatest technological importance.

In our previous and current work on this subject [18], [26], [27] we have been able to develop and verify the "germ" of these possibilities, but we have not had time to exhaustively study them. During the next two years we shall:

1. Thoroughly develop and implement the equations of our theory using the best computational resources available;
2. Use this numerical model to study optical resonance phenomena in general and the self-stabilizing photon locked states in particular;
3. Seek to quantify the conditions and, if possible, the particular physical systems in which photon locked polarization bistability might occur;
4. Finally, provide theoretical guidance to experimentalists in a search for physical realizations of our theoretical prediction.

We are in a very good position to accomplish the last objective because of the ongoing experimental research in optical resonance phenomena within the department and in the triangle area.

With the Sun 386i workstation (obtained with previous ARO support) we have been able solve the equations of the theory more than eight times faster than before and

consequently are able to study more atoms and scan much larger regions of the parameter space of optical phenomena. We are thus able to introduce and resolve interaction details unreachable in previous theories or on our earlier equipment with this theory. A substantial portion of our new understanding of optical resonance phenomena comes from our ability to watch the dynamical evolution of the fully quantum mechanical system in "real time" using a suitable graphical display. We will continue to require such sophisticated resources to complete the planned research. The physics department's growing network of Sun workstations and the planned optical fiber link to the national net backbones (which will also provide access to the Cray YMP being installed in the Research Triangle) will provide us with augmented computational ability as required by the problem, possibly with a small additional investment on our part.

There is a real opportunity in this research not only to advance science but also to impact a frontier technology: information processing with a spatial (device) resolution of nanometers and a temporal (switch time) resolution of picoseconds or less.

Recent Work Published Under ARO Support

1. "Stress Dependence of the Chemical Potential of Adsorbates", M. Ciftan, V. Ruck, and E. Saibel. *Sol. St. Comm.* **27**, 439 (1978)
2. "The Chemostress Coefficient", *Sol. St. Comm.* **27**, 435 (1978).
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4. "Multiple scattering and non-muffin-tin band theory", presented at the South-eastern Sectional meeting of the APS, November, 1980.
5. "The position space Green's function and its application to a non-muffin-tin band theory". Ph.D. dissertation; June 1982.
6. "Generalized non-muffin-tin band theory", R. G. Brown and M. Ciftan, *Phys. Rev.* **B27**, 4564 (1983).
7. "Stress activated Raman scattering and microcrack detection", M. Ciftan, R. G. Brown, and E. Saibel, *Int J. Eng. Sci* **21**, 128 (1983).
8. "Dynamical Approach to Superradiance through Vacuum Instability", V. Benza, E. Montaldi and M. Ciftan, *Lett. Nuov. Cim.* **36**, 103 (1983).
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10. "A numerical application of a generalized non-muffin-tin band theory", Poster presented at Sanibel Quantum Chemistry Symposium, March, 1984.
11. "A generalized non-muffin-tin theory of band structure", R. G. Brown and M. Ciftan, *Int. J. Quan. Chem.: QCS* **18** ed. P. O. Lowdin, J. R. Sabin, M. C. Zerner. Wiley and Sons, New York, 1984.
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13. "Numerical tests of high-precision multiple-scattering band theory", R. G. Brown and M. Ciftan, *Phys. Rev.* **B33**, 7937 (1986).
14. "Convergence properties of an exact band theory", R. G. Brown and M. Ciftan, *Condensed Matter Theories* **1**, ed. F. B. Malik, Plenum, New York, 1986.

15. "Pseudospin-ordered optical bistability for two-level atoms", presented at the meeting of the SESAPS in Williamsburg, VA, November 1986.
16. "Critical Temperature Changes in Many-Layer Films and Between Plates", J. L. Han and M. Ciftan, *Phys. Lett. A* **124**, 495, 1987.
17. "Three-dimensional-two-dimensional Crossover Onset in Critical Dynamics of Classical Fluids", *J. Phys. C* **21**, 2641 (1988).
18. "Local dynamics, correlation, and phase transitions: N-body versus nonlinear quantum optics", R. G. Brown and M. Ciftan *Condensed Matter Theories* **3**, ed. J. S. Arponen, R. F. Bishop and M. Manninen, Plenum, New York, 1988.
19. "Generalized non-muffin-tin multiple scattering theory", R. G. Brown, *J. Phys. B* **21** (letter), L309 (1988).
20. "Multipolar integral equation theory and generalized multiple scattering theory", R. G. Brown and M. Ciftan *Condensed Matter Theories* **4**, ed. J. H. Keller, Plenum, New York, in press.
21. "Multipolar expansions in the empty lattice problem", R. G. Brown and M. Ciftan, *Phys. Rev. B* **15** (February, 1989).
22. Comment on "Energy band equations for a general periodic potential", R. G. Brown and M. Ciftan, *Phys. Rev. B* **15**, May 15 1988, in press.
23. "The multipolar integral equation method", R. G. Brown. Internal publication, being prepared for submission.
24. "Multipolar expansions in the empty lattice problem II", R. G. Brown and M. Ciftan, submitted to *Phys. Rev. B*.
25. "The N-atom optical Bloch equations: A microscopic theory of quantum optics", R. G. Brown and M. Ciftan - manuscript submitted to *Phys. Rev. A* 4/20/88.
26. "Polarization Bistability", R. G. Brown and M. Ciftan - manuscript being prepared for submission.

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